New scenario for high-T_c cuprates : electronic topological transition as a motor for anomalies in the underdoped regime.

F. Onufrieva , P. Pfeuty, M. Kisselev
Laboratoire Leon Brillouin CE-Saclay 91191 Gif-sur-Yvette France

We have discovered a new nontrivial aspect of electronic topological transition (ETT) in a 2D free fermion system on a square lattice. The corresponding exotic quantum critical point, δ=δ_c, T=0, (n=$1-\delta$ is an electron concentration) is at the origin of anomalous behaviour in the interacting system on one side of ETT, $\delta < \delta_c$. The most important is an appearance of the line of characteristic temperatures, $T^*(\delta) \propto \delta_c - \delta$. Application of the theory to high-T_c cuprates reveals a striking similarity to the observed experimentally behaviour in the underdoped regime (NMR and ARPES).

This is a particularly exciting time for high-T_c. The experimental knowledge converges. Almost all experiments, NMR [1,2], ARPES [3], infrared conductivity [4] etc. provide an evidence for the existence of a characteristic energy scale $T^*(\delta)$ in the underdoped regime (δ is hole doping). Below and around the line $T^*(\delta)$ the "normal" state (i.e. above T_c) has properties fundamentally incompatible with the present understanding of metal physics. The field has reached the point when a consistent theory is necessary to understand this exotic from theoretical point of view but quite well defined from experimental point metallic behaviour. The issue has a significance beyond the field of high-T_c superconductivity - the fundamental question arises : what kind of metallic behaviour is there, in addition to the well understood Fermi liquid?

In the paper we propose our variant of the answer. We reexamine a free electron 2D system on a square lattice with hopping beyond nearest neighbors. We show that when varying the electron concentration defined as $1-\delta$, the system undergoes an electronic topological transition (ETT) [5] at a critical value δ=δ_c. The corresponding T=0 quantum critical point (QCP) combines several aspects of criticality. The first standard one is related to singularities in thermodynamic properties, in density of states at ω=0 (Van Hove singularity), to additional singularity in the superconducting (SC) response function (RF) [6]. The second nontrivial aspect is: the same QCP **is the end of the critical line** T=0, $\delta > \delta_c$ each point δ of which is characterized by static Kohn singularity (KS) in polarizability of 2D free fermions. [What we mean as a static KS is a singularity at the wavevector connecting two points of Fermi surface (FS) with parallel tangents [7]]. The two aspects of criticality are not related with each other. It is the latter aspect (never considered before) which as we will show is a motor for anomalous behaviour in the regime $0 < \delta < \delta_c$ of the system of noninteracting and interacting electrons (or of any fermion-like quasiparticles e.g. of those [8] appearing in the $t-t'-J$ model describing the strongly correlated CuO_2 plane responsible for main physics in the cuprates). The found anomalies have a striking similarity to anomalies in the underdoped high-T_c cuprates. The effect exists in all cases $t' \neq 0$ or/and $t'' \neq 0$ ... except for special sets of the parameters corresponding to the perfect nesting in FS (including t'=t''=...$\rightarrow$ 0) studied in many papers, see e.g. [9]. For such sets the QCP loses the latter aspect of criticality and the anomalies disappear.

A starting point is a 2D electron system on a square lattice with hopping beyond nearest neighbors

$$\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - ... \quad (1)$$

For any set of the parameters t, t', t'',... the dispersion law is characterized by two different saddle points (SP's) located at $(\pm\pi, 0)$ and $(0, \pm\pi)$ with the energy ϵ_s. When we vary the chemical potential μ or the energy distance from the SP, $Z = \mu - \epsilon_s$, the topology of the FS changes when Z goes from $Z > 0$ to $Z < 0$ through the critical value $Z = 0$. In vicinities of SP's the dispersion law is :

$$\tilde{\epsilon}(\mathbf{k}) = \epsilon_{\mathbf{k}} - \mu = -Z + ak_\alpha^2 - bk_\beta^2, \quad (2)$$

where $\mathbf{k}$ is measured from $(0, \pi)$ ($\alpha = x$, $\beta = y$) or from $(\pi, 0)$ ($\alpha = y$, $\beta = x$). Explicit expressions for a and b depend on t, t',... We consider the general case : $a \neq 0$, $b \neq 0$, $a \neq b$. We choose $a > b$ corresponding to $t'/t < 0$.

The $T = 0$ ETT has several characteristic aspects. The first (trivial) one is related to the **local change of FS topology** in the vicinity of SP. This leads to divergences in thermodynamic properties, in density of states at $\omega = 0$ etc. From this point of view the corresponding QCP is of a gaussian type with the dynamic exponent $z = 2$.

The nontrivial aspect is related to **mutual change** in topology of FS in vicinities of two different SP's and reveals itself when considering the electron polarizalibility

$$\chi^0(\mathbf{q}, \omega) = \frac{1}{N} \sum_{\mathbf{k}} \frac{n^F(\tilde{\epsilon}_{\mathbf{k}}) - n^F(\tilde{\epsilon}_{\mathbf{q+k}})}{\tilde{\epsilon}_{\mathbf{q+k}} - \tilde{\epsilon}_{\mathbf{k}} - \omega - i0^+}. \quad (3)$$

We show that the latter has a square-root singularity at ω=0 and wavevector $\mathbf{q}$=$\mathbf{q}_m$ in a vicinity of $\mathbf{Q}$=(π, π) **for any Z on the semiaxis** $Z < 0$: $\chi^0(\mathbf{q}, 0) - \chi^0(\mathbf{q}_m, 0) \propto \sqrt{|\mathbf{q}_m - \mathbf{q}|}$ for $\mathbf{q} < \mathbf{q}_m$. It is a static KS in the 2D electron system. The locus of the wavevectors $\mathbf{q}_m$ in the BZ is a closed curve around $\mathbf{Q}$ with $|\mathbf{Q} - \mathbf{q}_m| \propto \sqrt{|Z|}$. With decreasing $|Z|$ the closed curve shrinks and is reduced to the point $\mathbf{q} = \mathbf{Q}$ at $Z = 0$ where $\chi^0(\mathbf{q}, 0)$ diverges logarithmically. The curve of the static KS's with $\mathbf{q}$ close

to $\mathbf{Q}$ does not reappear for $Z > 0$: $\chi^0(\mathbf{q}, 0)$ is peaked at $\mathbf{q}$=$\mathbf{Q}$ in an intimate vicinity of ETT and it exhibits a wide plateau around $\mathbf{q} = \mathbf{Q}$ for larger Z. To illustrate this we show in Fig.1 the $\mathbf{q}$ dependence of $\chi^0(\mathbf{q}, 0)$ calculated based on (3) and (1). [We use the model with only $t' \neq 0$ being a generic model for the family: $a \neq 0$, $b \neq 0$, $a \neq b$.] The discussed above curve is the closest to $\mathbf{q} = \mathbf{Q}$ curve of singularities in Fig.1a. In the plots one sees only a quarter of the picture around $\mathbf{q} = \mathbf{Q}$; to see the **closed** curve around (π, π) one has to consider the extended BZ. [Few other curves of KS's seen in Fig.1 are not sensitive to ETT, we discuss them elsewhere.]

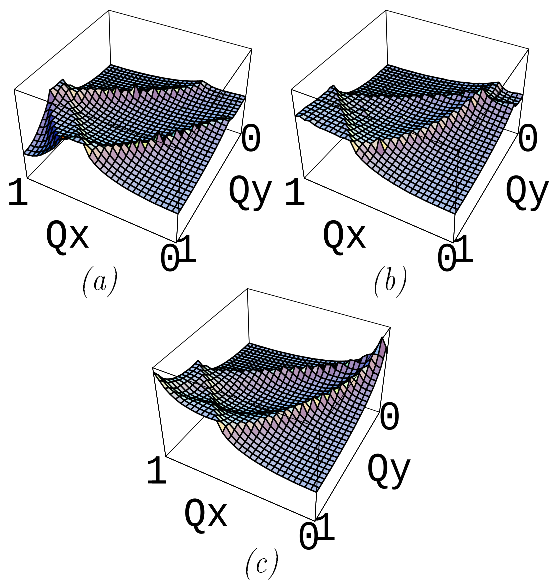

FIG. 1. $\mathbf{q}$ dependence of $\chi^0(\mathbf{q}, 0)$ through the Brillouin zone for (a)$Z < 0$, (b)$Z > 0$, (c)Z=0. Q_x=q_x/π, Q_y=q_y/π. The point $\mathbf{q} = \mathbf{Q}$ corresponds to the left corner. $(t'/t = -0.3)$

As a result, the point $Z = 0$, $T = 0$ turns out to be the end point of the critical line $Z < 0$, $T = 0$.

Paradoxically, the **absence** of the discussed curve of static KS's for $Z > 0$ leads to anomalous behaviour of the system on this side of QCP. To see this let's calculate ω dependencies of $Re\chi^0(\mathbf{q}, \omega)$, $Im\chi^0(\mathbf{q}, \omega)$ and $C(\omega)$=$Im\chi^0(\mathbf{q}, \omega)/\omega$ for the characteristic for this regime wavevector $\mathbf{q}$=$\mathbf{Q}$. Results are shown in Fig.2a. One can see that all functions are singular at some energy ω_c.

Calculations with the hyperbolic spectrum (2) give the following expression: $Im\chi^0(\mathbf{Q}, \omega) = F(\omega/\omega_c, b/a)/2\pi t$, $Re\chi^0(\mathbf{Q}, \omega) = Re\chi^0(\mathbf{Q}, \omega_c) - \Phi(\omega/\omega_c, b/a)/t$ with

$$F(x, y) = \begin{cases} \ln \frac{\sqrt{1+xy}+\sqrt{1+x}}{\sqrt{1-xy}+\sqrt{1-x}}, & 0 \leq x \leq 1 \\ \ln \frac{\sqrt{1+xy}+\sqrt{1+x}}{\sqrt{x(1-y)}}, & x \geq 1 \end{cases}$$

$$\Phi(x, y) = \begin{cases} \gamma_1(y)(1 - x^2), & x - 1 < 0 \\ \gamma_2(y)\sqrt{x-1}, & 0 \leq x - 1 \ll 1 \end{cases} \tag{4}$$

$(\gamma_{1,2}(y) \ll 1)$. The **new energy scale** which appears and corresponds to the singularities in Fig.2a is given by

$$\omega_c = Z(1 + b/a).$$

The singularities at $\omega = \omega_c$ are dynamic 2D KS's.

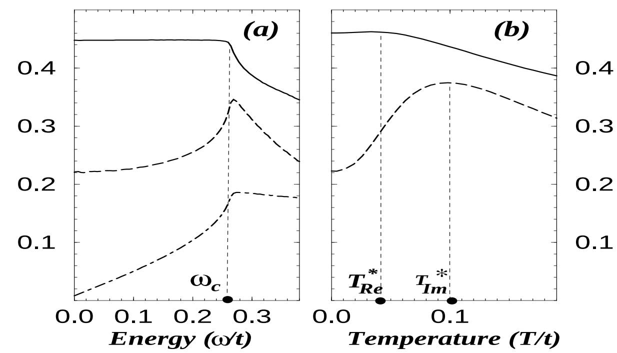

FIG. 2. $Re\chi^0(\mathbf{Q}, \omega)$ (solid), $Im\chi^0(\mathbf{Q}, \omega)$ (dot-dashed) and $C(\omega)$=$Im\chi^0(\mathbf{Q}, \omega)/\omega$ (dashed) in the regime $Z > 0$ (a) as a function of ω for $T = 0$, (b) as a function of T for $\omega \to 0$ $(Im\chi^0(\mathbf{q}, 0) = 0)$. Here $t'/t = -0.3$, $Z/t = 0.21$.

The dynamic KS's at $T = 0$ are transforming into static Kohn anomalies at finite temperatures which again scale with Z, see Fig.2b. When comparing with Fig.2a one can see that the behaviour is similar being smoothed by the effect of finite T (both behaviour are very different from the standard one for noninteracting system). The important difference is that the characteristic temperatures of the Kohn anomalies for $Re\chi^0(\mathbf{Q}, 0)$ and for $\lim_{\omega\to 0} Im\chi^0(\mathbf{Q}, \omega)/\omega$ being both scaled with Z

$$T^*_{Re} = AZ, \quad T^*_{Im} = BZ, \quad A < B$$

are different on the contrary to the characteristic energy of the KS's at T=0 (that is an usual effect of finite T).

Another remarkable signature of **asymmetry in** Z is the following. Taken for the characteristic for each regime wavevector, $\mathbf{q}$=$\mathbf{q}_m$ for Z< 0 and $\mathbf{q} = \mathbf{Q}$ for $Z > 0$, $\chi^0(\mathbf{q}, 0)$ decreases rapidly with $|Z|$ for Z< 0 (ordinary behaviour) while for Z> 0 it remains **practically constant** (and quite high) for Z not too small. Moreover for finite T, $\chi^0(\mathbf{Q}, 0)$ has a maximum at Z=$Z^*(T)$> 0 (that is very unusual). As a result of the described T and Z dependencies of $\chi^0(\mathbf{Q}, 0)$ in the regime $Z > 0$, the lines $\chi^0(\mathbf{Q}, 0)$=const have an unusual form in the $T - Z$ plane: they develop rather around the "critical" lines $T^*_{Re}(Z)$ and $T^*_{Im}(Z)$ than around the QCP, T=0, Z=0.

On the contrary, a behaviour of SC RF (in both cases isotropic s-wave or d-wave symmetry) is symmetrical in Z being related to the first aspect of ETT. For the same reason the SC RF decreases quite rapidly with increasing a distance from QCP, i.e. with increasing T and $|Z|$.

Above we considered a system of noninteracting electrons. In fact the same picture takes place for any system of fermion or fermion-like quasiparticles which dispersion law is determined by the topology of 2D square lattice and has a form (1). In [8] where we discuss some problems

of strongly correlated systems we show that such quasiparticles (with spin and charge) do exist in the $t-t'-J$ model describing the strongly correlated CuO_2 plane. On the other hand, the shape of FS observed by ARPES does imply the existence of nnn hopping $t' \neq 0$, so that the condition of the asymmetry $a \neq b$ necessary for the existence of the discussed ETT is fulfilled. Moreover this shape implies $t'/t < 0$, the case for which the critical doping δ_c is positive. Below we will pass from the energy distance from ETT, Z, to the doping distance, $\delta_c - \delta$, using large FS condition: $1-\delta = 2\sum_{\mathbf{k}} n^F(\tilde{\epsilon}_{\mathbf{k}})$ [8].

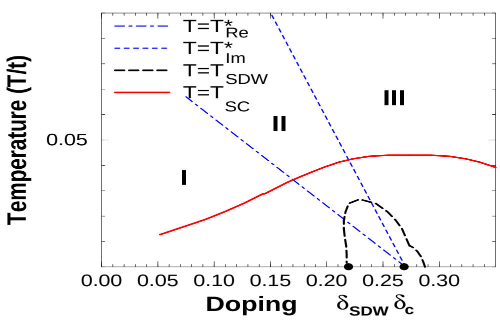

FIG. 3. Phase diagram with the lines of SDW and d-wave SC instabilities and the lines $T^*_{Re}(\delta)$, $T^*_{Im}(\delta)$ ($t'/t = -0.3$, $t/J = 1.9$). We consider only the metallic part of phase diagram (for discussion about a passage from AF localized-spin state at low doping to the metallic state with large FS for intermediate doping see [8]).

Let's consider now the system in the presence of interaction. A quite trivial consequence of the ETT is a developing of density wave (DW) and SC instabilities around the point $\delta{=}\delta_c$, $T{=}0$. [The effects are related to the logarithmic divergence of $\chi^0(\mathbf{Q},0)$ and $\ln Z \ln T$ divergence of the SC RF as $T \to 0$, $Z \to 0$.] Nontrivial consequences concerning the DW degrees of freedom and related to the Kohn singularity aspect of ETT are: *(i) strong asymmetry between regimes $\delta < \delta_c$ and $\delta > \delta_c$ and (ii) very long (in doping and temperature) memory about DW instability in the disordered state on one side of ETT, $\delta < \delta_c$*. To see this let's consider the electron-hole RF which in the simplest RPA approximation is given by $\chi(\mathbf{q},\omega) = \chi^0(\mathbf{q},\omega)/(1+V_{\mathbf{q}}\chi^0(\mathbf{q},\omega))$. In the case of interaction $V_{\mathbf{q}}$ in a triplet (singlet) channel the instability and normal state fluctuations are of SDW (CDW) type. We will consider the former interaction: $V_{\mathbf{q}}{=}J_{\mathbf{q}}{=}2J(\cos q_x + \cos q_y)$ ($J>0$) as strongly supported by neutron scattering and NMR experiments for the cuprates and on the other hand as an interaction between the discussed above quasiparticles in the $t{-}t'{-}J$ model [8]. For such interaction both instabilities d-wave SC (see details in [8]) and SDW take place around QCP. Due to the symmetry of SC RF in Z, $T_{sc}(\delta)$ is symmetrical on two sides of δ_c with a maximum at $\delta = \delta_c$, see Fig.3. Therefore the regimes $\delta < \delta_c$ and $\delta > \delta_c$ can be considered as underdoped and overdoped, respectively. On the contrary, the line of SDW instability, $T_{SDW}(\delta)$, given by $\chi^0(\mathbf{q},0) = -1/J_{\mathbf{q}}$ ($\mathbf{q}=\mathbf{Q}$ for $\delta < \delta_c$ and $\mathbf{q}=\mathbf{q}_m$ for $\delta > \delta_c$) has an anomalous form in the regime $\delta < \delta_c$: it develops rather around the lines $T^*_{Re}(\delta)$ and $T^*_{Im}(\delta)$ than around QCP (see Fig.3) reproducing the form of lines $\chi^0(\mathbf{Q},0) = const$ discussed above.

When at certain doping, $\delta{=}\delta_{SDW}$, the ordered SDW solution disappears, it is the disordered metallic state which keeps this type of behaviour: the regime $T^*_{Re}(\delta) < T < T^*_{Im}(\delta)$ (II) turns out to be a regime of a **minimum disorder** and the regime $T < T^*_{Re}(\delta)$ (I) a regime of **a reentrant in temperature quantum SDW liquid**. Indeed, two most important parameters characterizing SDW liquid: $\kappa^2 = 1 - |J_{\mathbf{Q}}|\chi^0(\mathbf{Q},0)$ describing a "proximity" to the SDW instability and $\Gamma_{\mathbf{Q}} = \kappa^2/C(0)$ describing a relaxation energy behave in a reentrant way in increasing T: κ^2 decreases (slightly) with T until $T^*_{Re}(\delta)$ and $\Gamma_{\mathbf{Q}}$ decreases (strongly) until $T^*_{Re}(\delta) < T^*_{\Gamma} < T^*_{Im}(\delta)$ as if the system would move towards an ordered phase. However, it does not reach it, the reentrancy stops and the system passes to the regime II of a minimum disorder above which a standard disordered state behaviour is restored (regime III). On the other hand, the quantum SDW liquid state in the regime I is practically **frozen in doping** due to the very weak dependence of κ^2 on doping. As a result the disordered metal state in the regime $\delta < \delta_c$ keeps a strong memory about the ordered SDW phase (and therefore develops strong critical SDW fluctuations) very far in doping and in temperature. On the contrary, in the regime $\delta > \delta_c$ the memory about SDW instability and the corresponding fluctuations disappear rapidly due to the sharp decrease of $\chi^0(\mathbf{q},0)$ with increasing $\delta - \delta_c$ and T. The same is valid in both regimes $\delta > \delta_c$ and $\delta < \delta_c$ for SC fluctuations due to the discussed in the first part behaviour of SC RF as a function of T and $|Z|$. Therefore, although the SDW phase itself is energetically unfavorable with respect to the SC phase (except of the case of very high J/t), the metal state above T_{sc} in the underdoped regime is a precursor of the SDW phase rather than of the SC phase.

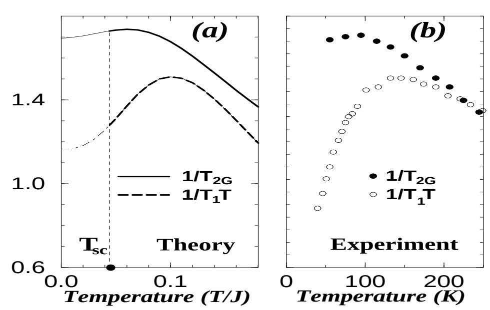

FIG. 4. $1/T_1T$ and $1/T_{2G}$ (a) calculated for $\delta = 0.15$ ($t'/t = -0.3$, $t/J = 1.9$) (should be considered only above T_{sc}) and (b) taken from NMR for $YBCO_{6.6}$ [2].

The lines $T^*_{Re}(\delta)$ and $T^*_{Im}(\delta)$ are basic lines for anomalies in the disordered metallic state. To demonstrate how the anomalies appear for different properties we consider some examples. In Fig.4a we show calculated quasistatic

magnetic characteristics corresponding to the measured by NMR $1/T_1T$ and $1/T_{2G}$ on copper as functions of T. A physical reason for a slight increase of $1/T_{2G}$ extending until $\approx T^*_{Re}$ and a much stronger increase of $1/T_1T$ extending until $T \approx T^*_\Gamma$ is the discussed above reentrant behaviour of κ^2 and $\Gamma_{\mathbf{Q}}$ with T. The theoretical behaviour is very close to that observed experimentally (Fig.4b) and explains it in fact for the first time.

In Fig.5 we show an electron spectrum calculated for the ordered SDW phase (a) and for the disordered metal state (namely for the regime II) (b). For the ordered phase the spectrum is given by: $\varepsilon_{1,2} = (\epsilon_A + \epsilon_B)/2 \pm \sqrt{(\epsilon_A - \epsilon_B)/2)^2 + \Delta^2}$ ($\epsilon_A(\mathbf{k}) \equiv \epsilon(\mathbf{k})$, $\epsilon_B(\mathbf{k}) \equiv \epsilon(\mathbf{k}+\mathbf{Q})$) with the gap Δ determined selfconsistently in the usual way. For the disordered state the "spectrum" is obtained from maxima of electron spectral functions strongly renormalized due to interaction with the described above SDW fluctuations. The characteristic form of the spectrum in both cases is a result of a hybridization of two parts of the bare spectrum in the vicinity of two different SP's $(0,\pi)$ and $(\pi,0)$. The hybridization is static for the ordered SDW phase and is dynamic for the disordered state. [Details about the pseudogap opening in the disordered state and its behaviour with T and δ will be a subject of a separate paper.] The spectrum is in excellent agreement with ARPES data, see Fig.5c (ARPES measures only the part corresponding to $\omega < 0$). The effect of splitting into two branches and of the pseudogap disappears quite rapidly in the regime $\delta > \delta_c$ due to the rapid weakening of SDW fluctuations. Due to the same reason it disappears roughly above $T^*_{Im}(\delta)$. Both facts agree with experiments for the cuprates.

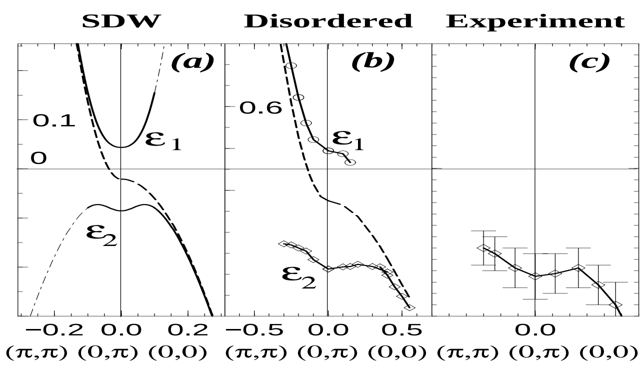

FIG. 5. Electron spectrum $\varepsilon(\mathbf{k})/t$ along $\Gamma - X$ symmetry lines, (a) in SDW phase (Z/t=0.03 (δ=0.25), T=0), (b) in the metallic state above T_{sc} (Z/t=0.3 (δ=0.1), T/t=0.15), (c) ARPES data [10] for underdoped $Bi_2Sr_2CaCu_2O_{8+delta}$ above T_{sc}. The dashed lines correspond to the bare spectrum, the thin line in (a) to the spectrum with the spectral weight less than 0.1. t'/t=−0.3, t/J=1.8, wavevectors are taken in unit of π.

Let's discuss a behaviour of $Im\chi(\mathbf{q},\omega)$, the characteristics measured by inelastic neutron scattering (INS). As follows from the previous analysis, below T^*_{Im} it has a maximum at ω=$\omega_0 \propto \kappa^2$ (being peaked at $\mathbf{q}$=$\mathbf{Q}$). So far as κ^2 almost does not change with δ, the position of the peak does not as well. This agrees with INS data and explains (for the first time) the existence of the characteristic energy ($\sim$ 30 meV) above T_{sc} for all δ, see e.g. the summarizing picture in Fig.25 in [11]. As was emphasized before, strong SDW fluctuations disappear in the overdoped regime $\delta > \delta_c$. In the underdoped regime they disappear (or strongly diminish) above $T^*_{Im}(\delta)$. Both facts are in a good agreement with INS.

Summarizing, the simple picture arising from the effect of ETT in 2D electron system on a square lattice gives a unified vision of normal state anomalies in the underdoped high-T_c cuprates for both magnetic and electronic properties. We succeed to explain the temperature anomalies in $1/T_1T$ and $1/T_{2G}$ NMR characteristics, some crucial features of INS in the normal state, the disappearance of magnetic fluctuations in the overdoped regime, an opening of a pseudogap in electron spectrum, the shape of the latter in a vicinity of $(0,\pi)$, the disappearance of the pseudogap in the overdoped regime. All these are most nontrivial experimental results. Regarding that the theory does not use any external phenomenological hypothesis and only two microscopical parameters t'/t and t/J, the similarity between the theoretical results and experiments seems quite remarkable. We emphasize that the effect exists for any t'/t, t''/t,... except of two limit cases: (i) isotropic one a=b in eq.(2) (t'=t''=...=0) and (ii) extreme anisotropic one a=0 or b=0. Although ETT exists in both cases, the corresponding QCP's belong to different classes of universality. For a=b (nesting) the behaviour is symmetrical in Z, the anomalous regime discussed in the paper disappears.

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